Development of an Adaptive Non-Ideal MHD Simulation Tool for Multiple Space Science Applications
Progress report

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1 Introduction

Over the last 16 years our group at the University of Michigan has been developing a general use global MHD code, BATS-R-US, and the Space Weather Modeling Framework (SWMF) that couples domain models extending from the Sun to planetary upper atmospheres and ionospheres. BATS-R-US and the SWMF have been extensively used to simulate a broad range of space science phenomena. Still there are many unmet challenges. There is a need to go beyond ideal MHD and to improve the efficiency of the numerical schemes.

In the first year of this AISRP we have developed

- finished and published the Hall MHD scheme
- added an electron equation to the MHD equations
- added a multi-ion MHD equation module
- tested the empirical resistivity model by M. Kuznetsova

In the second year we have

- added the electron pressure gradient term to Hall MHD
- finished the multi-ion MHD implementation and published a paper
- implemented a prototype for the time-accurate local time stepping algorithm
- started work on the non-isotropic pressure

- implemented a new algorithm to reduce the numerical diffusion

Our systematic studies of the non-gyrotropic model indicate that it is unlikely to produce physically correct results for complex and realistic magnetospheric simulations. Once the sawtooth oscillations are started, they continue even when the physical parameters in the solar wind do not justify the presence of the oscillations (according to observations). For this reason we have decided not to pursue the generalization of the non-gyrotropic model to the non-symmetric case.

Below we will describe the developments performed in the second year of the project in more detail.

1.1 Electron pressure gradient in Hall MHD

The Hall MHD equations have been implemented with explicit and implicit time stepping, on Cartesian and generalized block-adaptive grids. The code scales well to many hundreds of processsors. The details of the algorithm and a series of tests have been published in the Journal of Computational Physics (G. Toth, Y. J. Ma, T. I. Gombosi, 2008, JCP, 227, 6967-6984). Some applications have also been published (3D global multi-Species Hall-MHD simulation of the Cassini T9 flyby, Y. J. Ma et al, 2007, Geophysical Research Letters, 34, L24S10).

We have recently added the electron pressure gradient term into the generalized Ohm's law:

$$\mathbf{E} = -\mathbf{u}_e \times \mathbf{B} + \eta \mathbf{J} - \frac{\nabla p_e}{e n_e} \tag{1}$$

where $\mathbf{u}_e = \mathbf{u} - \mathbf{J}/(e\, n_e)$ is the electron velocity, $\mathbf{u}$ is the bulk velocity, $\mathbf{B}$ is the magnetic field vector, $\mathbf{J}$ is the current density, η is the resistivity, $-e$ is the charge of the electron, n_e is the electron number density, and p_e is the electron pressure. The new term is the last one. Since the electric field is needed at the cell faces in the induction equation $\partial \mathbf{B}/\partial t = -\nabla \times \mathbf{E}$, we have to discretize the electron pressure gradient at the cell faces. This is quite challenging at resolution changes. We use the same discretization techniques as developed for the Hall term, where $\mathbf{J} = \nabla \times \mathbf{B}$ has to be calculated at the cell interfaces. The algorithm is described in the 2008 JCP paper.

The electron pressure p_e is either approximated as a fixed fraction of the ion pressure, or we solve the electron pressure equation:

$$\frac{\partial p_e}{\partial t} + \nabla \cdot (\mathbf{u}_e p_e) = -(\gamma - 1) p_e \nabla \cdot \mathbf{u}_e + \eta \mathbf{J}^2 + S(p_e) \tag{2}$$

Note that the Joule heating is present in the electron pressure equation, but it is negligible (due to a coefficient of electron mass per ion mass) in the ion pressure equation. $S(p_e)$ represents arbitrary source terms, including the ion-electron collisional heat exchange term in case of non-negligible classical resistivity.

An interesting test of the electron pressure gradient term is the generation of magnetic field from zero initial conditions. This is the only term that can

generate $\mathbf{B}$ from "nothing". The initial conditions are $\mathbf{B} = 0$, $\mathbf{u} = 0$, $n_e = n_0 + n_1 \cos(k_x x)$ and $p_e = p_0 + p_1 \cos(k_y y)$. The resulting magnetic field is

$$\frac{\partial B_z}{\partial t} = \frac{k_x k_y n_1 p_1 \sin(k_x x) \sin(k_y y)}{(n_0 + n_1 \cos k_x x)^2} \tag{3}$$

Our test used $k_x = k_y = \pi/10$, $n_0 = p_0 = 1$ and $n_1 = p_1 = 0.1$ on a $|x|, |y| \leq 10$ periodic domain. We have successfully verified that the code reproduces the analytic solution with the expected order of accuracy.

Adding this term completes the implementation of the two-fluid Hall MHD equations into BATSRUS.

1.2 Multi-ion MHD equations

We have finished the implementation of the multi-ion MHD equations. The gradient of the electron pressure was missing in the preliminary implementation, this is now corrected. The momentum equation for the ion fluid s is now written as

$$\frac{\partial \rho_s \mathbf{u}_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + I p_s) = n_s q_s (\mathbf{u}_s - \mathbf{u}_+) \times \mathbf{B} + \frac{n_s q_s}{n_e e} (\mathbf{J} \times \mathbf{B} - \nabla p_e) + S_{\rho_s \mathbf{u}_s} \tag{4}$$

where q_s and n_s are the charge and number density of the ion fluid s, respectively, and $\mathbf{u}_+$ is the charge weighted average of the ion velocities.

We have used the multi-fluid code to model the magnetosphere including the oxygen outflow from the ionosphere. The outflow can be specified as a constant flow with fixed densities and velocities for the two fluids, or we can use the Polar Wind Outflow Model (PWOM) to provide these quantities at the inner boundary of the magnetosphere model (BATS-R-US). The results have been written up in a paper that has been accepted by the Journal of Geophysical Research: "Multi-Fluid BATS-R-US: Magnetospheric Composition and Dynamics During Geomagnetic Storms, Initial Results" by A. Glocer, G. Toth, Y. Ma, and T. Gombosi.

We are also applying the multifluid MHD code to Mars. This work is done by Dalal Najib (graduate student), Andrew Nagy and Gabor Toth. In the Mars ionosphere there are four ion fluids (hydrogen, atomic oxygen, molecular oxygen and carbon dioxide) and we employ a spherical grid. We have made substantial progress but there are still some issues that need to be resolved.

1.3 Time-accurate local time-stepping

We have implemented a preliminary algorithm that uses different time steps in different blocks, yet the whole simulation advances in a time-accurate manner. The prototype algorithm mainly follows the ideas described in "An explicit multi-time-stepping algorithm for aerodynamic flows" by H. van der Ven, B.E. Niemann-Tuitman, and A.E.P. Veldman, Journal of Computational and Applied Mathematics 82, 423 (1997). The basic idea is to calculate the smallest of the

stable time steps in each block, then update a "master clock" with this time step, but advance blocks with a locally stable time step when their individual time falls behind the master clock. The ghost cells of the blocks are interpolated in time.

For sake of parallel efficiency the block time steps are rounded down to integer powers of 2 times the smallest time step. This creates relatively few groups of blocks with identical time steps (i.e. they are advanced at the same time) which makes load balancing much easier. It also makes the flux-correction step much simpler to implement than in case of arbitrary time steps that can overlap arbitrarily. In fact, the Berger and Colella scheme (that employs time steps proportional to the cell size of the AMR grid) can be regarded as a special case of the above algorithm.

We also plan to allow local time step adjustments during the global time step in case stability requires. This may be required if the solution changes a lot in a single global time step. This may slightly offset the load balancing, but will avoid stability issues.

The prototype implementation demonstrates second order accuracy and stability with local time steps on two levels of an AMR grid. The local CFL number is the same (0.8) as for the fixed time step algorithm. The flux correction step and load balancing will be implemented soon.

1.4 Non-isotropic pressure

We have started work on the MHD equations with non-isotropic pressure. As a first step we have implemented a new equation module with an extra parallel (with respect to the magnetic field) pressure variable in addition to the usual MHD variables. We will solve for the parallel and total pressures. The orthogonal pressure can be obtained as a derived quantity. The next step will be adding the flux and source terms.

1.5 New algorithm for reduced numerical diffusion

Although it was not part of the original AISR proposal, we have implemented a new algorithm that fits nicely into the physics and algorithmic improvements of the project.

The basic idea actually comes from the Hall MHD algorithm developed in the first year of this project. We noticed that in an implicit time stepping scheme one can reduce or even ignore the numerical diffusion associated with the whistler wave speed, and this can greatly increase the accuracy of the scheme, while the oscillation-free property is still maintained as long as there are no fast whistler waves present in the simulation.

The same idea can be applied to ordinary MHD. One can use an implicit time stepping and limit the diffusive numerical flux to some well chosen maximum speed. For example in a magnetosphere simulation, one may limit the wave speed used in the numerical flux to 2000 km/s. Our numerical experiments show that the numerical code remains stable, and the numerical diffusion is

greatly reduced. The effect is similar to the Boris correction with an artificially reduced speed of light, but there are two distinct differences:

- The MHD equations are not modified by the flux limiting, only the numerical scheme. The Boris correction with the reduced speed of light changes the equations.
- The flux limiting can be employed in the Roe scheme too, while the Boris correction cannot.

We plan to publish a short note on this scheme and the obtained results in the near future with Xing Meng (graduate student), Gabor Toth and Tamas Gombosi.